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2. REPORT DATE	January 14, 1993
3. REPORT TYPE AND DATES COVERED	Annual Report 10/15/91 - 10/14/92
4. TITLE AND SUBTITLE	Optoelectronics Based on SiGe/Si Heterostructures
5. FUNDING NUMBERS	AFOSR-91-0313 CR
6. AUTHOR(S)	Kang L. Wang
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	University of California, Los Angeles Electrical Engineering Dept. 66-147B Engineering IV Bldg. 405 Hilgard Ave. Los Angeles, CA 90024-1594
8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	AFOSR/NE Building 410 Bolling AFB, Washington DC 20332-6448
10. SPONSORING/MONITORING AGENCY REPORT NUMBER	2305CS
11. SUPPLEMENTARY NOTES	
12a. DISTRIBUTION/AVAILABILITY STATEMENT	Approved for public release, distribution unlimited

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13. ABSTRACT (Maximum 200 words)

The overall objective of the research is to explore SiGe/Si heterostructures for optoelectronic applications. In addition to exploration of new devices, alternative growth techniques for achieving layer thickness to monolayer scale and doping control are also investigated. We have discovered a new transition at normal incidence for p-type quantum well structures, in addition to previously observed intersubband transition. One of the advantages of this intervalence band transition is the detection of infrared at normal incidence. The application of these transitions for the fabrication of tunable normal incidence infrared detectors have also demonstrated. We have also demonstrated normal incidence intersubband transition in the conduction band of SiGe/Si quantum wells grown on (110) Si substrate due to the nonvanishing off-diagonal elements of the effective mass tensor. In the area of transport properties, we have studied the in-plane mobility of coupled δ-doped quantum wells as a function of spacing between the wells. An enhancement of hole mobility above that of the Si was found due to the penetration of wavefunctions into the spacer where the impurity scattering is minimal. In the area of the growth control of SiGe epitaxial layers, we have modified a MBE system for handling the gaseous species for gas beam epitaxy study.

14. SUBJECT TERMS	Heterostructures Strain Relaxation Intervalence Band Optoelectronics Intersubband
15. NUMBER OF PAGES	15
16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT	Unclassified
18. SECURITY CLASSIFICATION OF THIS PAGE	Unclassified
19. SECURITY CLASSIFICATION OF ABSTRACT	Unclassified
20. LIMITATION OF ABSTRACT	UL

Air Force Office of Scientific Research

Annual Technical Report

For the Period

July 1, 1991 to September 30, 1992

for

Optoelectronics Based-on SiGe/Si Heterostructures
(Contract AFOSR-91-0313)

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List of Figures

1 Statement of Work

The overall objective of the research is to explore SiGe/Si heterostructures for optoelectronic applications. In addition to exploration of new devices, alternative growth techniques for achieving layer thickness to monolayer scale and doping control are also investigated. The role of surfactants on the epitaxial growth is to be investigated, in particular, for obtaining high quality coherently strained SiGe films and for providing doping control in quantum wells and superlattices. In the following, we highlight the accomplishments made both in the growth control and optoelectronic properties. Details may be referenced to the publications resulting from the research efforts under the AFOSR support listed in the Appendix.

2 Status of the Research Effort

In the following sections, we will describe the accomplishments made on growth and optoelectronic device application of strained $Si_{1-x}Ge_x/Si$ heterostructures. We have discovered a new transition at normal incidence for p-type quantum well structures, in addition to previously observed intersubband transition. The strength of this transition is shown to depend strongly on the Ge composition in the well. For low Ge compositions only the intersubbannd transition is observed. One of the advantages of the intervalence band transition is the detection of infrared at normal incidence. The normal incidence detection is prohibited in the cases of intersubband (same Bloch function) transition occurred at the Γ-valley. The application of these transitions for the fabrication of tunable normal incidence infrared detectors have also demonstrated.

We have also demonstrated normal incidence intersubband transition in the conduction band of SiGe/Si quantum wells. The principle for such normal incidence detection is attributed to the nonvanishing off- diagonal elements of the effective mass tensor. The off-diagonal elements of the effective mass tensor occur only if the structure is grown on a selected substrate orientation, for example, on Si (110) or (111) orientation. The data on structures grown on Si (110) substrate clearly indicate that indeed such a transition is possible if the strain in the quantum well is properly adjusted. In the area of transport properties, we have studied the in-plane mobility

of coupled δ- doped quantum wells as a function of spacing between the wells. An enhancement of hole mobility above that of the Si was found due to the penetration of wavefunctions into the spacer where the impurity scattering is minimal. In the area of the growth control of SiGe epitaxial layers, we have modified a MBE system for handling the gaseous species for gas beam epitaxy study. This will allow the control of the growth by chemical reaction instead of simply having physical processes involved in the MBE. This can potentially solve the problems of doping as well as the control of layer thickness allowing the fabrication of doping superlattices for optoelectronic applications. We have also made significant advances in the understanding of optical properties of strained SiGe layers as well as intersubband transitions of $Si_{1-x}Ge_x/Si$ multiple quantum wells including the importance of many-body effects in determining the absorption peak position.

In the following we will give a concise discussion on the tasks accomplished in the past year.

2.1 δ-doped Quantum Wells and Many-Body Effects

The understanding of heavy doping on the intersubband transitions is important for tuning the detection wavelength of quantum well infrared detectors. In the study we have used δ-doped quantum wells in Si. The key point is to show that the many-body effects due to δ-doping can be used to tune the transition energy, independent of effective mass. The δ-doping in semiconductors can be viewed as an alternative way of achieving quantum well structures without heterojunctions. The well thickness and the barrier height can be controlled by the thickness of the doped layer and the doping density.

A typical structure used in this study consists of an undoped Si buffer layer, followed by 10 periods of 35 Å of heavily boron-doped Si layers and 300 Å of undoped Si spacers. Figure 1 shows the (SIMS) depth profile for a typical δ-doped structure (sample A). A full width at half maximum (FWHM) of approximately 50 Å is obtained from the depth profile.

Measured absorption spectra of samples with different doping densities as a function of photon energy are shown in Fig. 2. It can be clearly seen that the absorption

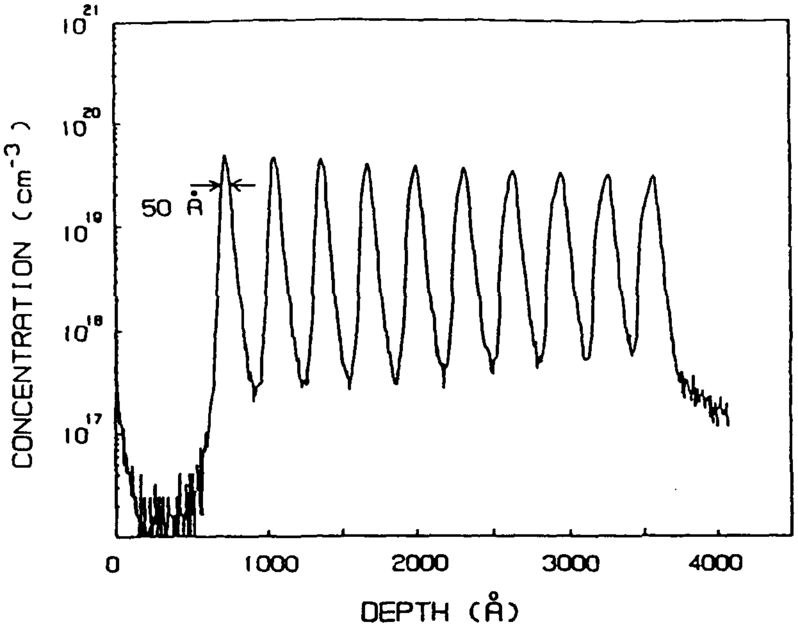


Figure 1: SIMS depth profile of sample A. It reveals 10 periods of boron δ-doped Si layers with a FWHM of about 50 Å.

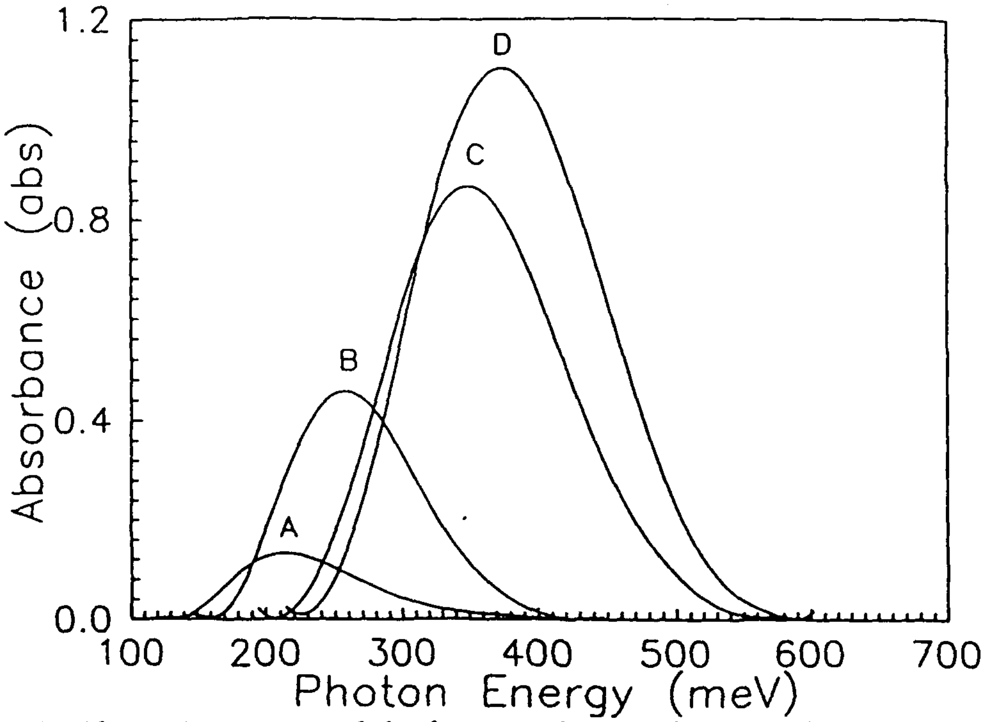


Figure 2: Absorption spectra of the four samples as a function of photon energy at 300 K. The set of curves are due to different doping concentrations.

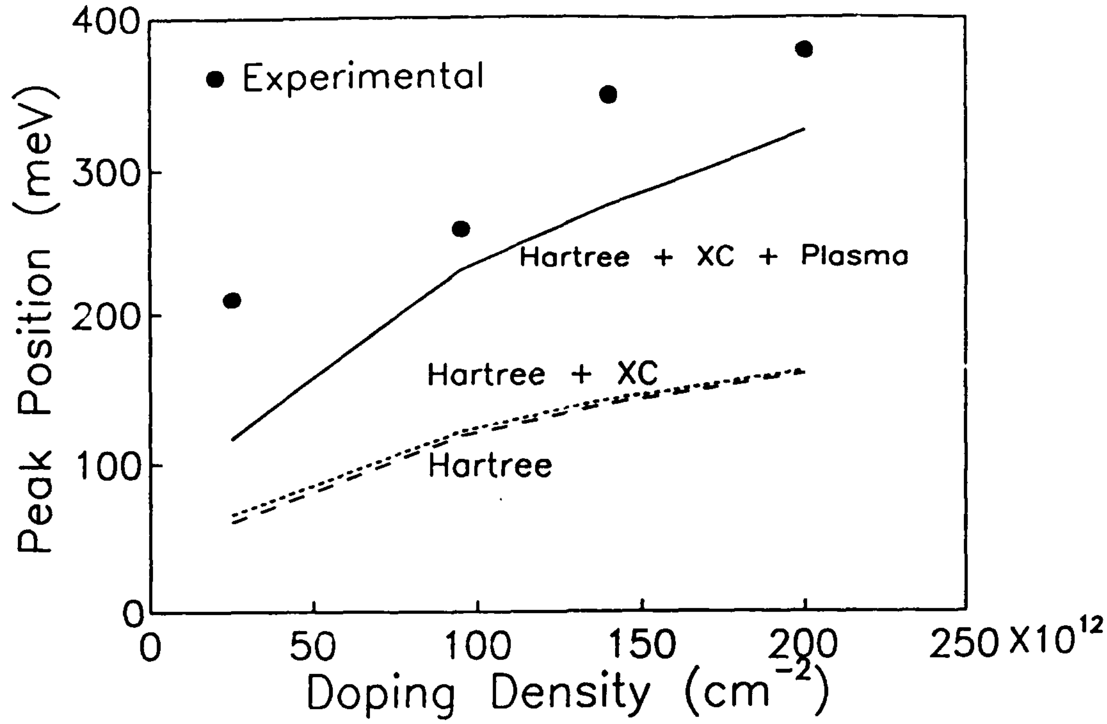


Figure 3: Subband separation as a function of doping density (a) experimental data (solid circles), (b) using the Hartree approximation (dashed curve), and (c) using many-body effects including exchange-correlation, depolarization and excitonic interactions (solid curve).

spectra shift towards the high energy regime with increasing absorption as the doping density is increased. The shift of the absorption peak is mainly due to the enhancement of depolarization effect as well as increase of the potential well depth at high doping densities. The widths of the absorption peaks are more than an order of magnitude larger than those observed in GaAs/AlGaAs quantum well structures, typically about 10 meV. The polarization dependence of the spectra shows a similar behavior as in the case of multiple quantum wells.

The potential profile and the energy level spectrum in the well is usually obtained by solving the Schrödinger's and Poisson's equations self-consistently using the exchange-correlation potential in the density-functional approximation. The experimental peak position along with the calculated values using a multi-band self-consistent calculation (dashed-curve) are shown in Fig. 3. These values are considerably smaller than the experimental values shown by the solid circles. The solid curve in the Fig. 3 shows the calculated results by incorporating many-body effects (i.e., exchange-correlation, depolarization and excitonic like interactions). This brought the calculated and experimental peak positions to a reasonably close agreement. Similar

behavior have also been observed in the case of intersubband transitions in heavily doped SiGe/Si quantum well structures. This work demonstrate for the first time the importance of many-body effect in tuning of the transition energy. The situation does not happen in the case of GaAs quantum wells as the effective mass and the density of states is substantially lower to have significant effect.

2.2 Normal Incidence Intersubband Absorption

One of the major drawbacks of intersubband transition is that the normal incidence light cannot be detected. In order to circumvent this limitation, we have studied the normal incidence intersubband transitions in both n-type and p-type SiGe/Si MQWs. For n-type, this results from the coupling of light with the off-diagonal components of the electron effective mass tensor, or the tilted energy ellipsoids being away from the Γ-point. The intersubband absorption at the Γ-point requires a component of photon electric field along the quantum well direction. For the (100) oriented Si substrate the condition applies since the (100) directions lie in the principal directions of the constant energy ellipsoids. On the other hand, for a similar structure grown on a (110) Si substrate, the non-zero off- diagonal effective mass components provide the coupling of normal incident light to induce the intersubband transition. Figure 4 shows the intersubband absorption in δ-doped quantum wells for (100) and (110) oriented substrates. The polarization dependence absorption data for the structure grown on (110) Si substrate confirms the normal incidence transition. Next, we will discuss similar transitions in the valence band due to band mixing.

For p-type, with a significant band coupling from the conduction Γ-point, it is possible to have transition between different hole bands (for example, between the heavy and light hole bands). This is particularly important in the case of SiGe grown on Si substrate where the strain reduces the bandgap resulting in a strong coupling between the conduction and valence bands as the Ge composition is increased. The evaluation of the optical matrix element using $\mathbf{k}\cdot\mathbf{p}$ approximation indicates the strength of this transition is inversely proportional to the square of the bandgap which, reduces as the Ge composition is increased.

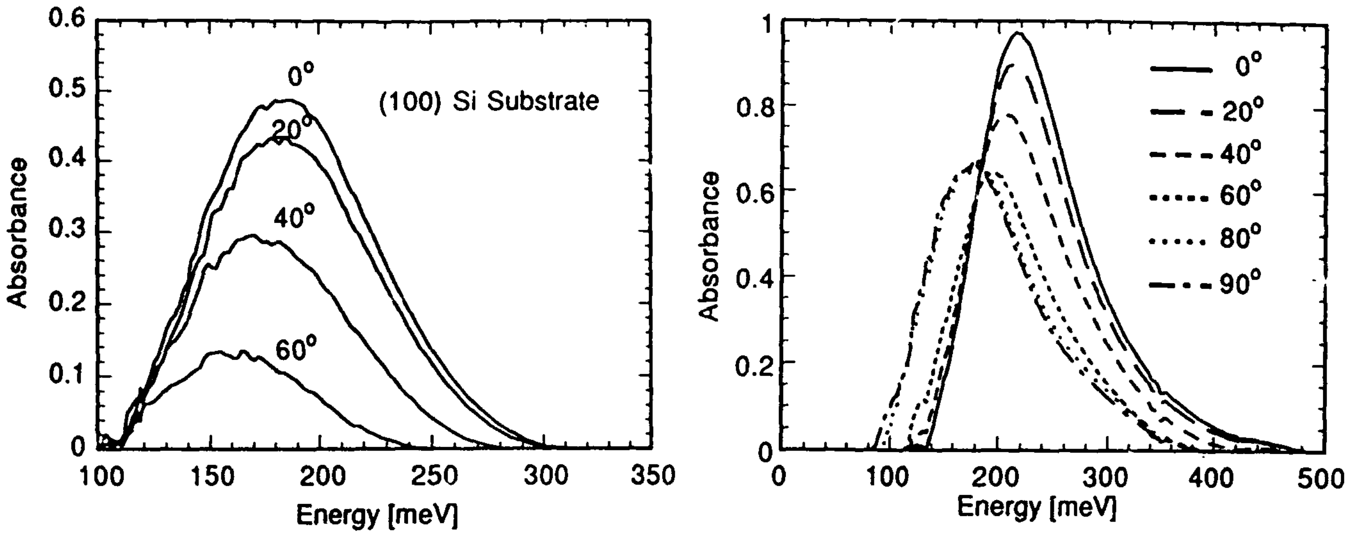


Figure 4: Intersubband absorption by δ-doped structures grown on (100) and (110) oriented Si substrates. The polarization dependence data of (110) structure shows the normal incidence absorption.

In the experiment, two $Si_{1-x}Ge_x/Si$ multiple quantum well structures with 30% and 60% Ge compositions was employed. Figure 5 shows the room temperature absorption spectra at the 90° polarization (i.e., normal incidence) for the two samples as a function of wavelength using a 45° multipass waveguide structure, 5 mm long and 0.5 mm wide. For clarity, we have subtracted the monotonically increasing background absorption mainly due to free carrier absorption in the doped quantum wells. The magnitude of the observed absorption coefficient ($\sim 10^4$ cm^{-1}) is as large as typically observed in direct gap semiconductors. As shown in Fig. 5, peaks in the absorption were observed at 3.4 and 2.5 μm for samples 30% and 60%, respectively. This normal incidence absorption is mainly due to excitation of holes from the heavy hole ground state to the ground state of the split-off band and the continuum hole subbands. The enhancement of the absorption with increasing Ge composition is due to the reduction of the bandgap at the Γ-point as mentioned before.

Our research shows that normal incidence intersubband transition can be obtained for both n and p-type SiGe/Si quantum wells. The work also leads to further advance in the understanding of intersubband transition.

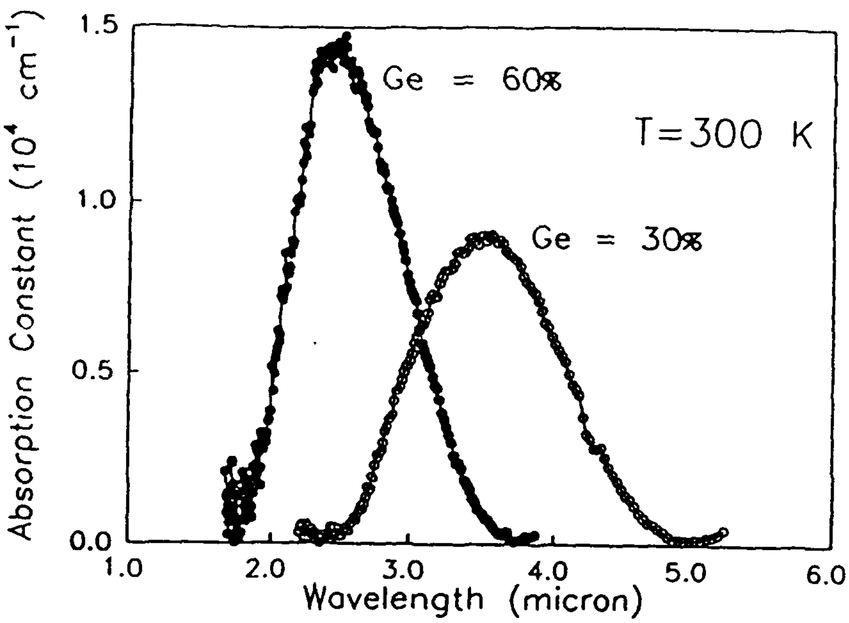


Figure 5: Intervalence band transition as a function of wavelength for two samples with different Ge compositions. The shift of the peak position is due to the splitting of the hole bands due to strain.

2.3 Detector Application

We have also investigated the potential of intervalence band absorption described above for normal incidence infrared detector application. The use of Si-based quantum well structures has an added advantage due to the potential for integrating with Si signal processing electronics in a monolithic manner. For the photoresponse measurement, mesa diodes of 200 μm in diameter were fabricated as schematically shown in the inset of Fig. 6. Infrared was illuminated on the mesa at normal incidence from the backside of the wafer. Figure 6 shows the responsivity (A/W) as a function of wavelength at 77 K for the two samples. It can be clearly seen from the measured result that as the Ge composition is increased the peak photoresponse moves towards a shorter wavelength, in agreement with the absorption data shown in Fig. 5. In comparison with the absorption data at room temperature, the photoresponse shows several peaks while the absorption spectrum has only one broad peak for either sample. The origin of these peaks are due to transition between the heavy hole ground

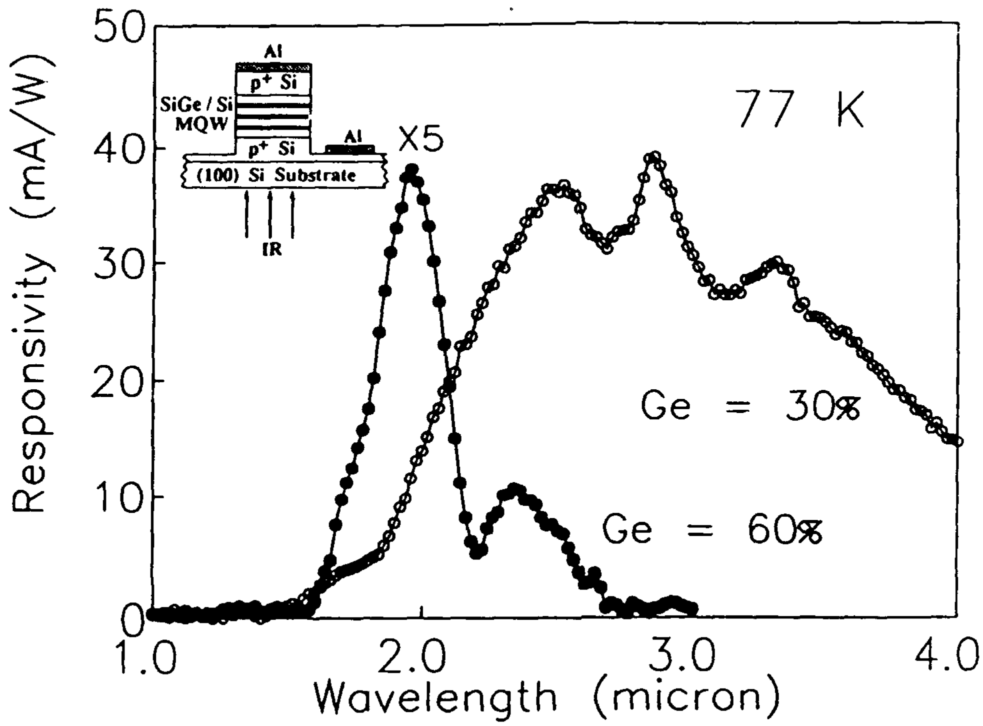


Figure 6: Measured responsivity at 77 K as a function of wavelength for a 200 μm mesa diode. Infrared is incident from the backside of the wafer (normal to the substrate plane) as shown in the inset.

state to the split-off ground state and the continuum hole states above the barrier. This has been further confirmed by using bias dependent photocurrent measurement.

2.4 Transport Properties of δ-doped Quantum Wells

Methods to increase the mobility and at the same time the carrier density, or conductance, are extremely important for enhancing the speed and frequency performance of devices. The purpose of the on-going research is to investigate various avenues such as strain, modulation doping, and δ doping in order to achieve higher mobilities with high carrier concentrations. One of the approaches employed was to use very thin heavily doped layers or referred to as coupled δ-doped quantum wells. We have found that when two or more of these wells are placed in close proximity with one another (on the order 200 Å) significant mobility enhancement results due to the fact that the central regions act like a modulation doped structure, and that the wave functions of the layers are closely coupled to have a substantial overlap. An example of the enhancement is shown in Fig. 7. The temperature dependence of the mobility for a

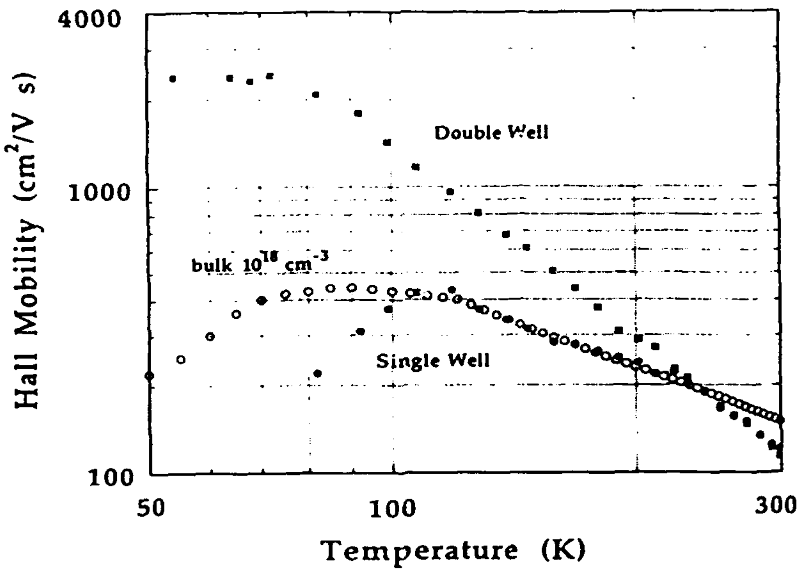


Figure 7: Hall mobilities as a function of temperature for the single δ layer, double δ layer, and Si bulk samples. The mobility enhancement is evident especially at lower temperatures.

bulk layer doped to 10^{18} cm^{-3} is also shown for comparison. The curve for the single well closely follows that of the bulk case as expected, showing Coulomb scattering at lower temperatures. Yet, the mobility of the double well continues to increase, saturating at a value of $\sim$ 2500 cm^2/Vs. What is also important to note is that the carrier density of the double well is two times the single well (of 1x10^{12} cm^{-2}). Thus an enhanced mobility is realized and at the same time, the carrier density is increased two fold. This leads to an increase of conductance of the double well over that of the single well or bulk Si. There exists many promising applications for both n-type and p-type coupled δ-doped layers including δ-doped bipolar transistors and high mobility FET's.

2.5 Luminescence from Strained SiGe Layers

There is a considerable interest in achieving efficient Si-based light emitters for potential application in optoelectronic integrated circuits. One of the approaches in accomplishing the goal is to investigate and understand the luminescence of Brillouin zone folded states in short period superlattices. To date, photoluminescence (PL) mechanism in short period superlattices (SLs) resulting from zone folding remains in

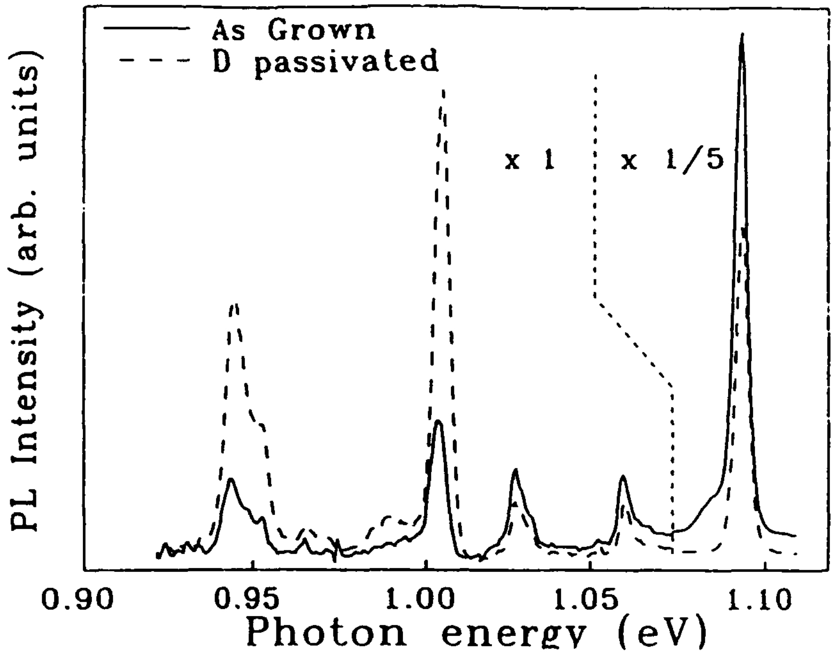


Figure 8: As-grown (solid line) and deuterated (dashed line) PL spectra of a $Si_{0.84}Ge_{0.16}$ alloy layer. The layer was passivated for 90 min. at 200 C.

debate. At the same time, the optical properties of pseudomorphic $Si_{1-x}Ge_x$ layers are still far from being fully understood. Therefore, in the past year, we examined the PL of thick $Si_{1-x}Ge_x$ strained layers grown by MBE on Si(100) oriented substrates. The sample used consists of a $Si_{1-x}Ge_x$ alloy layer capped with 3000 Å Si layer, both grown at low temperature. High resolution x-ray diffraction has been used to confirm that fully strained layers were achieved.

The PL spectrum of an as-grown 1600 Å thick $Si_{0.84}Ge_{0.16}$ alloy layer taken at 4.2 K is shown in Fig. 8. In the same figure, we show the PL spectrum of the sample after passivation with atomic deuterium (hydrogen). Deuterium is used for convenient SIMS analysis to be discussed later. The peaks at 1.027 eV, 1.060 eV, and 1.093 eV originate from the Si substrate. The peaks at lower energies correspond to the different types of participating phonons in the optical transitions originating from the alloy layer. The highest peak at ≈ 1.0 eV corresponds to a no-phonon bound exciton transition in which the alloy scattering of SiGe acts to conserve momentum. The difference in energies between the no-phonon line and the phonon assisted lines are in close agreement with the phonon energy values measured for the case of relaxed bulk alloy layers.

We have also performed atomic deuterium annealing in order to passivate the defect luminescence. (Atomic deuterium was created using a plasma discharge source and was used instead of hydrogen in order to reduce the background interference of hydrogen in SIMS analysis.) Upon deuteration, an enhancement of the SiGe peaks by a factor of more than three accompanied with a decrease in the intensity of the peaks coming from the Si substrate is apparent. These results demonstrate that for the relaxed case, the thick graded buffer layer is highly efficient in preventing the threading dislocations from propagating into the active layer and thus, quenching any type of excitonic luminescence. The progress is essential for the understanding of the optical properties of zone folded structures and is a major step for our long term objective of achieving efficient light emitters.

2.6 Gas Source MBE layered Material and Devices

In a step towards achieving ultimate growth control in an atomic layer- by-layer fashion, we have established the growth of Si and SiC using gas beam epitaxy (GBE). The deposition of Ge and Si by gas beams have not been performed to date owing to the safety regulation of the State and the Building in handling silane and germane. We will however set up such capability in the coming year. However, we have demonstrated the operation of the system by growing thin β-SiC film on Si-substrate at low temperature around 850 °C. β-SiC can be used to fabricate LED's for optical interconnect application. The growth of β-SiC was performed using a two-step growth method. First, a thin buffer layer was formed by surface carbonization with the C_2H_2 gas beam to relieve a large lattice mismatch (about 20 %) between SiC (4.36 Å) and Si (5.43 Å). After the carbonization process, the Si molecular beam was turned on under the simultaneous irradiation of the C_2H_2 beam for the MBE SiC growth. We have studied the reaction kinetics of C_2H_2 gas with Si in order to understand the self- limiting processes. The C_2H_2 gas shows a useful self-limiting reaction for the atomic layer epitaxy (ALE) process, in that C_2H_2 gas rapidly reacts with the highly reactive Si-surface; after forming β-SiC on Si-surface, the reaction of C_2H_2 gas with Si rapidly drops and the reaction almost stops. Figure 9 shows the evolution of the

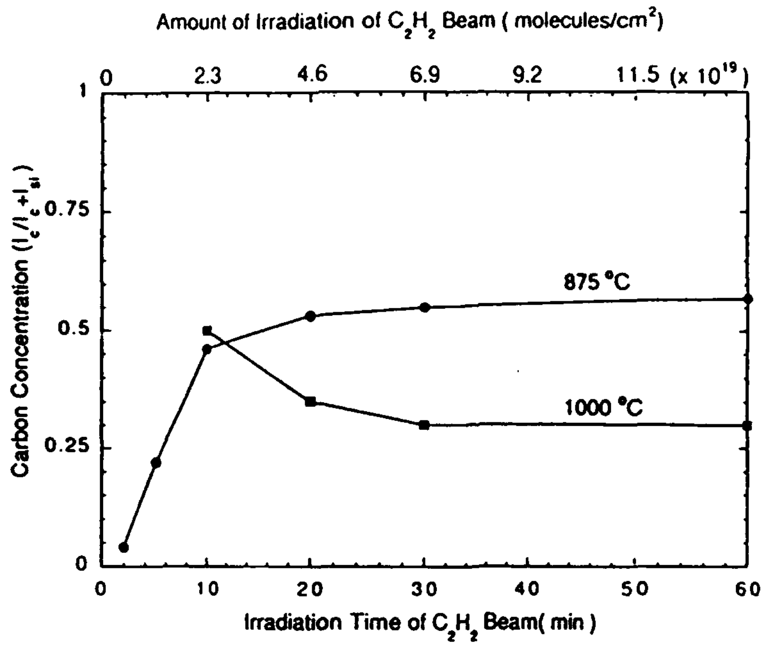


Figure 9: Evolution of the AES surface carbon concentration with irradiation of the C_2H_2 for 875 $^\circ C$ and 1000 °C substrate temperatures.

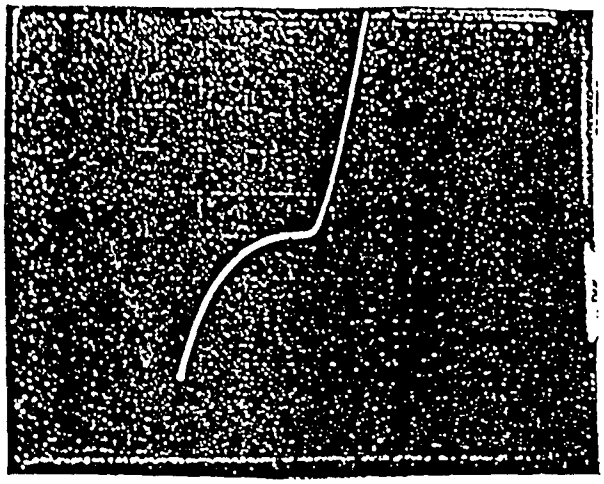
AES surface carbon concentration with exposure of irradiation of the C_2H_2 for two substrate temperatures at 875 °C and 1000 °C. As shown in Fig. 9, the ratio of C and Si concentrations (C/Si) at 875 °C carbonization temperature linearly increases from the pure Si- surface initially to presumably the formation of SiC (1:1 C/Si ratio) with the increase of the C_2H_2 beam exposure. This 1:1 C/Si ratio indicates the SiC stoichiometric composition. Further increase of the C_2H_2 beam irradiation does not seem to change the C/Si ratio. The thickness measurement of the SiC layer using ellipsometry shows that the saturation of the film thickness after 20 min of exposure occurs. From the AES and the thickness measurements, it is suspected that C_2H_2 gas rapidly reacts with the highly reactive Si- surface; after forming β-SiC on Si-surface, the reaction of C_2H_2 gas with Si drops rapidly and further reaction of SiC almost completely stops. Similar self-limiting reactions may be useful for group IV atomic layer epitaxy involving Si and Ge.

Electrical properties of the β-SiC films grown by this technique were studied using a hot thermal probe, I-V and C-V measurements. It is well known that an unintentionally doped β-SiC film on Si- substrate by CVD (chemical vapor deposition) gives

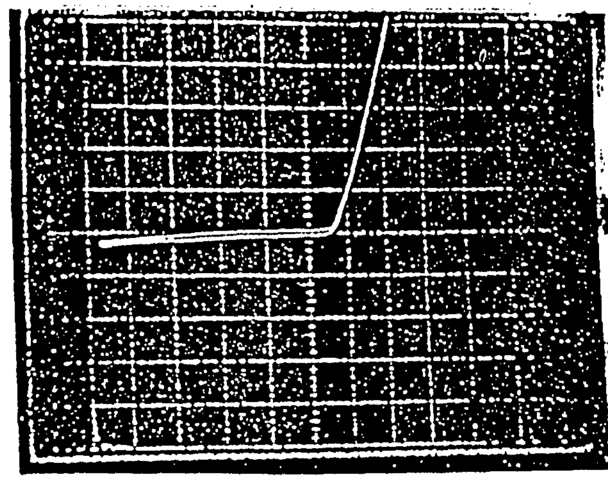
an n-type behavior having a residual donor concentration of 10^{16} cm^{-3}, regardless of Si substrate doping. The cause of this unintentional n-doping in β-SiC is not well established. Residual nitrogen doping from growth environment of CVD systems or nonstoichiometric defects were suggested. In our case, the unintentionally doped β-SiC films grown are almost intrinsic. To check the quality of SiC films for device application, we fabricated n/p diodes with thin a β-SiC layer. Figure 10 shows the I-V curves of diodes with and without the thin β-SiC film. The forward characteristics of p^+-n^+ diodes with and without the thin β-SiC layer are almost comparable. For p^+-n^+ diode without the β-SiC layer, a small reverse breakdown voltage due to tunneling between n^+ polysilicon and p^+ substrate was observed as shown in Fig. 10(a). The reverse breakdown voltage was improved by inserting a 100 Å thin undoped β-SiC as shown in Fig. 10(b). This work demonstrates the first step of gas MBE towards the ultimate of atomic layer epitaxy of Si and Ge. In the next step, we will explore the use of all gas beam for growth and eventually investigating the integration of SIC LED's on to Si VLSI. We will also begin the selective growth of strained layers of SiGe using GBE as soon as the Ge gas beam is introduced.

2.7 Summary

In summary, in the performance period we have explored the growth of group IV elements using gas source MBE to achieve better control of layer thickness and doping control. In the area of optical properties, we have studied the luminescence of strained SiGe layers. The luminescence originated from the alloy was discriminated from those of and dislocations using hydrogen passivation. We have also demonstrated normal incidence intersubband transitions in both n and p-type SiGe/Si multiple quantum wells. New understanding of intersubband transition has been attained. Potential application in normal incidence infrared detection is also demonstrated. In the study of transport properties we have demonstrated an enhancement of hole mobility of double δ- doped structures in Si due to coupling of wavefunctions.



(a)



(b)

Figure 10: I-V characteristics of (a) n^+(polysilicon)/p^+ diode, and (b) n^+(polysilicon)/β-SiC (100 Å)/p^+ diode. The scales are: current (0.1 mA/div) and voltage (1 V/div).

3 Publications in Technical Journals

Park, J. S., Karunasiri, R. P. G., and Wang, K. L., "Inter- valence-subband Transition in SiGe/Si Multiple Quantum Wells - Normal Incident Detection", Appl. Phys. Lett.,61, 681 (1992).

Karunasiri, R. P. G., Wang, K. L., and Park, J. S., "Intersubband Transitions in SiGe/Si Quantum Structures", Semiconductor Interfaces and Microstructures, World Scientific Publishing, pp 252-279 (1992)

Lee, Chanho and Wang, K. L., "Intersubband Absorption in Sb k- doped $Si/Si_{1-x}Ge_x$ Quantum Well Structures Grown on Si (110)", Appl. Phys. Lett., 60, 2264 (1992).

Karunasiri, R. P. G., Park, J. S., and Wang, K. L., "Normal Incidence Infrared Detector using Inter-valence-subband Transitions in $Si_{1-x}Ge_x$/Si Multiple Quantum Wells", to appear in Appl. Phys. Lett., 1992.

Wang, K. L., and Karunasiri, R. P. G., "Infrared Detectors Using SiGe/Si Quantum Well Structures", to be published (1993)

Carns, T. K., Zhang, X, and Wang, K. L., "Enhancement of Hall Mobility in Coupled δ-doped Wells", submitted to Appl. Phys. Lett. (1992).

Karunasiri, R. P. G., Wang, K. L., and Park, J. S., "Many-body Effect in Intersubband Transitions in δ-doped Si and SiGe Quantum Wells", submitted to Phys. Rev. B, 1992

Zhang, X, Carns, T. K., Wang K. L., and Wu, B. J., "Enhancement of Hall Mobility in Coupled δ-doped Layers Grown by MBE", submitted to Appl. Phys. Lett. (1992).

Tijero, J. M. G., Arbet-Engels, V., Manissadjian, A., Wang K. L., and Higgs, V., "Effect of Hydrogenation on the Luminescence of Strained $Si_{1-x}Ge_x$ Alloy Layers Grown by Molecular Beam Epitaxy", submitted to Appl. Phys. Lett. (1992).

4 Professional Personnel

K. L. Wang	Professor-Principal Investigator
Gamani Karunasiri	Assistant Research Engineer
Vincent Arbet-Engels	PhD student
Chenho Lee	PhD student
Timothy Carns	PhD student

5 Interactions

(i) Papers presented at meetings

Kim, K, Choi, S. D., and Wang, K. L., "Si-Heterojunction Diodes with Thin β-SiC Layer Prepared in Gas-Source MBE", 2nd International Symposium on ALE, Raleigh, North Carolina, June 2-5, 1992.

Carns, T. K., Zheng, X., and Wang, K. L., "Hole Mobility Enhancement in Double δ-doped Si Layers", to be presented at the North American Conference on Molecular Beam Epitaxy, Ottawa, Canada, October 12-14, 1992.

Karunasiri, R. P. G., Park, J. S., and Wang, K. L., "Normal Incidence Infrared Detector using Intervalence Band Absorption of $Si_{1-x}Ge_x$/Si Multiple Quantum Wells", 50th Annual Device Research Conference, June 22-24, 1992.

Karunasiri, R. P. G. and Wang, K. L., "MBE Growth and Optoelectronic Application of SiGe/Si Heterostructures", High Speed Optoelectronic Devices and Circuits II, Banff, Alberta, Canada, August 9-13, 1992.

Wang, K. L., "SiGe/Si Electronics and Optoelectronics", American Vacuum Society 39th Annual Symposium, Chicago, August 9-13, 1992.

Wang, K. L., "SiGe/Si Electronics and Optoelectronics—An overview", , China, August 9-13, 1992.

(ii) Consultive and advisory functions

We have interacted with Wright Laboratory of Air Force. We will help in preparation of several samples for their in-house research (Dr. William Mitchel). Similarly, discussions with Rome Air Force Labortary for SiGe IR detector application.